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Energy and Spectroscopic Characterization of the Isomers of $C_4H_3^-$, $C_6H_3^-$, and $C_6H_5^-$

Organic and inorganic molecules, neutral and ions have been observed in the interstellar medium. A few anions of organic molecules have also been observed recently. The Cassini spacecraft in the upper atmosphere of Titan has observed anions of large organic molecules. In this project we have studied the physical and spectroscopic properties of $C_4H_3^-$, $C_6H_3^-$, and $C_6H_5^-$. We have optimized the geometrical structures of all low-lying isomers of the anions, calculated rotational, and harmonic vibrational frequencies of the anions mentioned above using the B3LYP density functional along with the augmented correlation consistent polar valence triple zeta (aug-cc-pVTZ) basis set. We have found many low-lying isomers on the potential energy surface of these anions.